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FILE 'HOME' ENTERED AT 14:12:24 ON 12 APR 2003

=> file registry
COST IN U.S. DOLLARS
SINCE FILE ENTRY TOTAL
SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 14:12:41 ON 12 APR 2003
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 APR 2003 HIGHEST RN 502793-56-8
DICTIONARY FILE UPDATES: 11 APR 2003 HIGHEST RN 502793-56-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

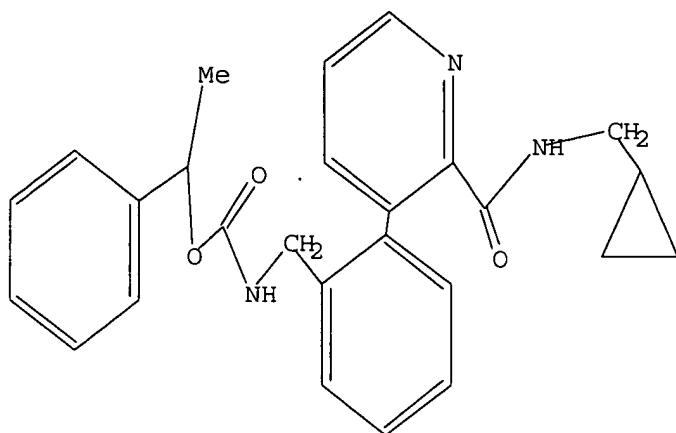
Crossover limits have been increased. See **HELP CROSSOVER** for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading 10002320.str

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 14:13:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5 TO 234

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 sss full

FULL SEARCH INITIATED 14:13:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 95 TO ITERATE

100.0% PROCESSED 95 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

FULL ESTIMATED COST

148.15

SESSION

148.36

FILE 'CAPLUS' ENTERED AT 14:13:20 ON 12 APR 2003
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FILE COVERS 1907 - 12 Apr 2003 VOL 138 ISS 16
FILE LAST UPDATED: 11 Apr 2003 (20030411/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 2 L3

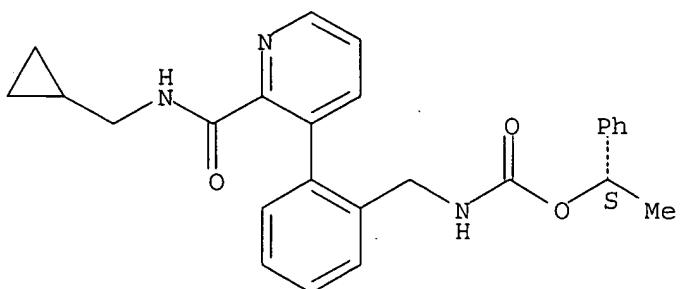
=> d 14 fbib hitstr abs total

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
AN 2003:49604 CAPLUS
TI Identification, Synthesis, and Activity of Novel Blockers of the Voltage-Gated Potassium Channel Kv1.5
AU Peukert, Stefan; Brendel, Joachim; Pirard, Bernard; Brueggemann, Andrea; Below, Peter; Kleemann, Heinz-Werner; Hemmerle, Horst; Schmidt, Wolfgang
CS Medicinal Chemistry and DG Cardiovascular, Aventis Pharma Deutschland GmbH, Frankfurt/Main, D-65926, Germany
SO Journal of Medicinal Chemistry (2003), 46(4), 486-498
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
IT 502169-87-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of o-[o-(aminomethyl)phenyl]arenecarboxamides as blockers of the voltage-gated potassium channel Kv1.5 and antiarrhythmic agents)
RN 502169-87-1 CAPLUS
CN Carbamic acid, [(2-[2-[(cyclopropylmethyl)amino]carbonyl]-3-pyridinyl]phenyl)methyl]-, (1S)-1-phenylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

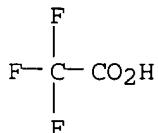
CM 1

CRN 434319-88-7
CMF C26 H27 N3 O3

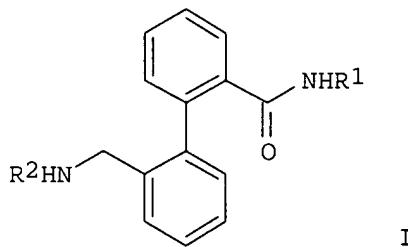
Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

GI



I

AB The voltage-gated potassium channel Kv1.5 is regarded as a promising target for the development of new atrial selective drugs with fewer side effects. In the present study, several ortho,ortho-disubstituted bisaryl compds., e.g. I [R1 = Me2CHCH2CH2, 2,4-F2C6H3CH2, 2-(2-pyridyl)ethyl, etc.; R2 = PhCH2OCO, 4-MeOC6H4CH2CO, PhCH2CH2, etc.] were synthesized and screened for their ability to block Kv1.5 channels expressed in Xenopus oocytes. The obsd. structure-activity relationship was described by a pharmacophore model that consists of three hydrophobic centers in a triangular arrangement. The hydrophobic centers are matched by a Ph or pyridyl ring of the bisaryl core and both ends of the side chains. The most potent compds. I [R1 = 2-(2-pyridyl)ethyl; R2 = PhCH2OCO, (S)-PhCHMeOCO] inhibited the Kv1.5 channel with sub-micromolar half-blocking concns. and displayed 3-fold selectivity over Kv1.3 and no significant effect on the HERG channel and sodium currents. In addn., compds. I [R1 = 2-(2-pyridyl)ethyl, R2 = PhCH2OCO; R1 = 2,4-F2C6H3CH2, R2 = 4-MeOC6H4CH2CO] have shown antiarrhythmic effects in a pig model.

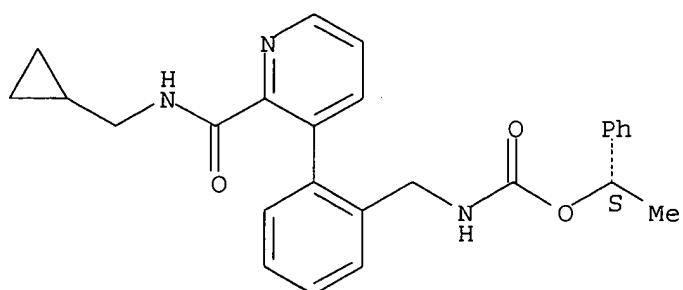
RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
 AN 2002:449654 CAPLUS
 DN 137:20388
 TI Preparation of ortho-substituted nitrogen containing bisaryl compounds as potassium channel blockers
 IN Peukert, Stefan; Brendel, Joachim; Hemmerle, Horst; Kleemann, Heinz-Werner
 PA Aventis Pharma Deutschland G.m.b.H., Germany
 SO PCT Int. Appl., 69 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002046162	A1	20020613	WO 2001-EP13680	20011124
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				DE 2000-10060807A 20001207
	DE 10060807	A1	20020620	DE 2000-10060807	20001207
	AU 2002021892	A5	20020618	AU 2002-21892	20011124
				DE 2000-10060807A 20001207	
				WO 2001-EP13680W	20011124
	US 2003060470	A1	20030327	US 2001-2326	20011205
				DE 2000-10060807A 20001207	
OS	MARPAT 137:20388				
IT	434319-88-7P				
	RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)				
	(prepn. of ortho-substituted nitrogen contg. bisaryl compds. as potassium channel blockers)				
RN	434319-88-7 CAPLUS				
CN	Carbamic acid, [(2-[2-[(cyclopropylmethyl)amino]carbonyl]-3-pyridinyl]phenyl)methyl]-, (1S)-1-phenylethyl ester (9CI) (CA INDEX NAME)				

Absolute stereochemistry.



GI

